

Thermodynamic properties of $d_{x^2-y^2} + id_{xy}$ Superconductor

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Abstract

In view of the current interest in $d_{x^2-y^2} + id_{xy}$ superconductors some of their thermodynamic properties have been studied to obtain relevant information for experimental verification. The temperature dependence of the specific heat and superfluid density show marked differences in $d_{x^2-y^2} + id_{xy}$ state compared to the pure d-wave state. A second order phase transition is observed on lowering the temperature into a $d_{x^2-y^2} + id_{xy}$ state from the $d_{x^2-y^2}$ state with the opening up of a gap all over the fermi surface. The thermodynamic quantities in $d_{x^2-y^2} + id_{xy}$ state are dominated by this gap as in an s-wave superconductor as opposed to the algebraic temperature dependence in pure d-wave states coming from the low energy excitations across the node(s).

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Introduction

The series of experiments carried out over the last few years to establish the nature of symmetry in high temperature superconductors with their level of sophistication and ingenuity have thrown up new challenges towards an understanding of the physics of these systems[1, 2]. New findings have come up with surprising regularity with the latest one being the observation of a plateau in the thermal conductivity by Krishana et al.[3] and its subsequent interpretation in terms of the appearance of a time-reversal symmetry breaking state ($d_{x^2-y^2} + id_{xy}$)[4].

An understanding of the pairing mechanism that underlies the superconducting instability is essential for the emergence of a microscopic theory for these superconductors. Countless experiments have been performed and various theoretical models have been proposed to probe the symmetry of the OP in these highly anisotropic unconventional superconductors. At present it is almost universally accepted that the OP is highly anisotropic with a symmetry of the d-wave[1].

In the recent experiment of Krishana et. al.[3] thermal conductivity as functions of both magnetic field and temperature has been measured on a sample of high T_c superconducting material $Bi_2Sr_2CaCu_2O_8$. They observed that the thermal conductivity initially decreases with the increase of magnetic field and above a particular value of the field, which depends on

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temperature, thermal conductivity becomes independent of field. These observations gave an indication that the material undergoes a phase transition in presence of the magnetic field. The authors suggested that this magnetically induced phase might have a complex order parameter symmetry such as $d_{x^2-y^2} + id_{xy}$ or $d_{x^2-y^2} + is$ where the gap is nonzero on the entire FS. Corroboration of these results came quickly from other groups as well[5].

Laughlin[4] showed that in presence of magnetic field the new superconducting phase must have an OP that violates both time reversal and parity and is of $d_{x^2-y^2} + id_{xy}$ symmetry. There were earlier predictions for such a state in the region near a grain boundary where the gap has sharp variation across it[6] with a spontaneous current generated along the boundary and in a doped Mott insulator with short range antiferromagnetic spin correlation[7, 8].

It would, therefore, be interesting to study the thermodynamic behaviour of such superconductors having OP symmetry of $d_{x^2-y^2} + id_{xy}$ type to provide further experimental observations to confirm its existence. We use the usual weak coupling theory to obtain the gap functions in the region of parameter space where a $d + id$ state is a stable one, and calculate thermodynamic quantities like the specific heat and superfluid density (and hence the penetration depth) and contrast them with a pure d-wave state.

Model and Calculations

Unlike pure d-wave OP, the $d_{x^2-y^2} + id_{xy}$ gap function has no node along the FS. The OP has non-zero magnitude all over but it changes sign in each quadrant of the Brillouin zone, while a pure s-wave OP does also have non vanishing magnitude but its sign remains same throughout. This non vanishing gap inhibits creation of quasiparticle excitations at low energies whereas in a pure d-wave state the gapless excitations are available in large numbers at low energies due to the presence of line nodes. Taking a tight binding model for a 2-dimensional square lattice, various physical quantities have been calculated within the framework of the usual weak coupling theory. The effective interaction has been taken in the separable form[9] and expanded in the relevant basis functions of the irreducible representation of C_{4v} .

$$V(\mathbf{k} - \mathbf{k}') = \sum_{i=1,2} V_i \eta_i(\mathbf{k}) \eta_i(\mathbf{k}')$$

where $\eta_1(\mathbf{k}) = \frac{1}{2}(\cos k_x - \cos k_y)$ and $\eta_2(\mathbf{k}) = \sin k_x \sin k_y$ (respectively for $d_{x^2-y^2}$ and d_{xy} symmetries). $V_1/8$ and $V_2/8$ are the respective coupling strengths for the near-neighbour and next near-neighbour interactions. The coupling strengths have been chosen in such a way as to allow both the components of the OP to exist simultaneously and the superconducting transition temperature of d_{xy} component to be lower than that of $d_{x^2-y^2}$ and is in the range of the observed values. Considering only the nearest neighbour hopping, the band dispersion is $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ where t is the nearest neighbour hopping integral and expanding the OP as $\Delta_{\mathbf{k}} = \sum_{i=1,2} \Delta_i \eta_i(\mathbf{k})$ for $\eta_i(\mathbf{k})$ defined above (for the $d_{x^2-y^2} + id_{xy}$ symmetry), the standard mean-field gap equation becomes a set of two coupled equations

$$\Delta_1 = -V_1 \sum_{\mathbf{k}} \frac{\Delta_1}{2E_{\mathbf{k}}} \eta_1^2(\mathbf{k}) \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right)$$

and

$$\Delta_2 = -V_2 \sum_{\mathbf{k}} \frac{\Delta_2}{2E_{\mathbf{k}}} \eta_2^2(\mathbf{k}) \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right).$$

Here the quasiparticle spectrum in the ordered state is given by $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta_{\mathbf{k}}|^2}$ where μ is the chemical potential. The coupled set of gap equations are solved numerically in a selfconsistent manner with the parameters $t = 0.15$ eV, $V_1 = 0.445t$ eV and $V_2 = 3.202t$ eV. The solutions give the expected square root temperature dependences of the two components of the order parameter $d_{x^2-y^2}(\Delta_1)$ and $d_{xy}(\Delta_2)$ and the corresponding T_c s (T_{c1} and T_{c2}) as shown in Fig. 1. It is to be noted that the consistent solutions exist for both $d_{x^2-y^2}$ and d_{xy} components of the OP for a very narrow range of V_1 and V_2 . The d_{xy} component of the OP exists only when the next nearest neighbour interaction (V_2) is taken into account. It has also been observed that the solutions have sensitive dependence on the values of the chemical potential and the next nearest neighbour hopping integral(t'). To be more specific, if we change the value of chemical potential to -0.25 eV from $\mu = 0$ with $t' = 0$, the $d + id$ state ceases to exist, but the inclusion of the t' term (with $t' = 0.4t$) brings the $d + id$ state back. The solutions, of course, exist only for a narrow range of values of the chemical potential: for instance $\mu = -0.22$ eV to $\mu = -0.26$ eV with $t' = 0.4t$ has well defined solutions with $\Delta_1(0) > \Delta_2(0)$. Similarly if we keep the value of μ fixed at any of the above values and start changing the value of t' , only a very narrow range of t' gives us a $d + id$ solution. This interplay of t' and μ is dictated by the location of the van Hove singularity (vHS) with respect to the fermi energy.

The quasiparticle spectrum along different directions in the first quadrant of the Brillouin zone is shown in Fig. 2 and the finite gap along all k -points is clearly visible. With the excitation spectrum thus obtained, it is straightforward to calculate thermodynamic quantities, namely, the specific heat and superfluid density, in the different ordered states. From the usual definition in terms of the derivative of entropy[10], we calculate the specific heat across the transitions and show it in Fig. 3. Two sharp jumps in the specific heat curve are observed at the respective transition temperatures.

The superfluid density $\rho_s(T)$ has been calculated using the standard techniques of many body theory[11, 12]. In the presence of a transverse vector potential with the chosen gauge $A_y = 0$, the hopping matrix element(t_{ij}) for the kinetic energy term in the Hamiltonian(H_0) is modified by the Peierl's phase factor $\exp[\frac{ie}{\hbar c} \int_{\mathbf{r}_j}^{\mathbf{r}_i} \mathbf{A} \cdot d\mathbf{l}]$. The total current (in the linear response) $J_x(\mathbf{r}_i)$ produced by the potential consists of both the diamagnetic and paramagnetic terms and can be derived by differentiating H_0 with respect to $A_x(\mathbf{r}_i)$. Hence

$$j_x(\mathbf{r}_i) = -c \frac{\partial H_0}{\partial A_x(\mathbf{r}_i)} = j_x^{para}(\mathbf{r}_i) + j_x^{dia}(\mathbf{r}_i)$$

where the paramagnetic current in the long wavelength limit in the linear response is given by

$$\mathbf{j}_x^{para}(\mathbf{q}) = -\frac{i}{c} \lim_{q \rightarrow 0} \lim_{\omega \rightarrow 0} \int d\tau \theta(\tau) e^{i\omega\tau} \langle [j_x^{para}(\mathbf{q}, \tau), j_x^{para}(-\mathbf{q}, 0)] \rangle \mathbf{A}_x(\mathbf{q}),$$

and the diamagnetic part is given by

$$\mathbf{j}_x^{dia}(\mathbf{q}) = -\frac{e^2}{N\hbar^2 c} \sum_{\mathbf{k}, \sigma} \langle c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \rangle \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial^2 k_x^2} \mathbf{A}_x(\mathbf{q}).$$

Here the averaging is done in the mean-field superconducting state. Fig. 4 shows the variation of ρ_s with temperature. At low temperatures where the superconductor is in $d_{x^2-y^2} + id_{xy}$ state, the superfluid density exhibits an exponential decay reflecting the gapped excitations. Above the second transition temperature (T_{c2}) at which the d_{xy} component of the OP vanishes and the superconductor undergoes a transition to $d_{x^2-y^2}$ phase, the superfluid density curve shows a power law behaviour expected from the low energy quasiparticles.

Results and Discussion

The self-consistent solutions for the order parameters (Fig. 1) show that as we decrease the temperature, first there is a continuous transition into a superconducting state where the OP is of $d_{x^2-y^2}$ symmetry with no d_{xy} component. On further decreasing the temperature a second continuous transition occurs and the d_{xy} component appears (with a phase $\pi/2$ with respect to the $d_{x^2-y^2}$ component) breaking the time reversal symmetry. A stable $d + id$ phase does not exist unless the next nearest neighbour interaction is being considered. This is because the next nearest neighbour attraction accounts for the pairing along the (110) direction. The sensitive dependence of the solutions on the chemical potential and the next near neighbour hopping integral is understood by studying the nature of the non-interacting density of states (DOS). It has been noticed that the van Hove singularity (vHS) in the non-interacting DOS lies far away from the fermi level when we include the t' term in the band keeping the chemical potential zero, but if in addition we change the the chemical potential to -0.25 eV, the vHS moves close to the fermi level.

In the $d_{x^2-y^2} + id_{xy}$ state there exists no node on the FS, a gap opens throughout. Hence the low energy quasiparticle excitations are exponentially down in comparison to the pure d-wave state that has line nodes on the FS. This is borne out from the plot of the quasiparticle energy spectrum along different directions of BZ (Fig. 2).

As temperature decreases from T_c corresponding to the $d_{x^2-y^2}$ state, the low energy quasiparticle excitations are exponentially low in the $d_{x^2-y^2} + id_{xy}$ state due to the appearance of an additional OP of d_{xy} symmetry and phased by 90 degree with the existing $d_{x^2-y^2}$ OP. The thermodynamic quantities are therefore affected in this new state quite severely. The temperature dependence of the specific heat (Fig. 3) shows the difference. The sharp jumps at transition temperatures in the specific heat curve, are clear indication of second order transitions[13]. The nature of the curve has significant difference in the two superconducting states (pure $d_{x^2-y^2}$ and the $d + id$). In the $d_{x^2-y^2} + id_{xy}$ state the specific heat increases exponentially with temperature, more like the familiar s-wave superconductors whereas in the d-wave state the growth is more stiff. This in turn indicates that the entropy is higher in pure d-wave state than that in $d_{x^2-y^2} + id_{xy}$ state. So the low temperature $d + id$ phase, in a way, is more ordered than the higher temperature $d_{x^2-y^2}$ phase.

The curve for the superfluid density as a function of temperature (Fig. 4) behaves differently in the two superconducting phases as expected. In the $d_{x^2-y^2} + id_{xy}$ phase ρ_s falls exponentially with temperature whereas in $d_{x^2-y^2}$ phase the descent is according to a power law. At the second transition temperature (T_{c2}), where the transition occurs between the two superconducting phases, a sudden upturn appears in the $\rho_s(T)$ curve which reflects the availability of quasiparticle excitations due to the disappearance of the d_{xy} state. If we compare these results with that of an s-wave superconductor, we observe that the behaviour of ρ_s in the $d_{x^2-y^2} + id_{xy}$ state is qualitatively similar to that of the s-wave state, with a gap all over the FS. Owing to this gap, the quasiparticle excitations are not easily accessible at very low temperatures and keeps the superfluid density almost independent of temperature at low temperatures. This exponential behaviour is expected in the thermodynamic properties whenever there exists a gap in the excitation spectrum.

In conclusion, the thermodynamic properties of the $d_{x^2-y^2} + id_{xy}$ superconductor are studied with a tight binding model within the mean-field theory. Significant differences have been observed in the nature of the temperature dependence of specific heat and superfluid density between a pure d-wave state and the $d_{x^2-y^2} + id_{xy}$ state. The behaviour in the latter is found to be somewhat similar to that of an s-wave superconductor. Further experimental observations on the thermodynamics of this state will shed light on the microscopic nature of interactions in these new class of superconductors.

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Figure captions

- Fig. 1. The gap parameters Δ_1 and Δ_2 (in Kelvin) versus temperature (in Kelvin).
- Fig. 2. The quasiparticle energy spectrum ($E_{\mathbf{k}}$) (in meV) along various symmetry directions in the first quadrant of BZ (the gap magnitudes have been increased ten times for visualisation). The inset shows how the symmetry directions are defined in BZ.
- Fig. 3 The specific heat versus temperature curve in $d_{x^2-y^2} + id_{xy}$ and $d_{x^2-y^2}$ states clearly shows the difference in its behaviour in these two states. The dotted line shows the normal state specific heat.
- Fig. 4 The superfluid density is shown against temperature for two phases $d_{x^2-y^2} + id_{xy}$ and $d_{x^2-y^2}$.







